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Block Predictor-Corrector Schemes for the Parallel Solution of ODEs

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Abstract—A fourth-order block method based on the composite Simpson rule is developed for the parallel solution of ordinary differential equations. Like the block scheme based on the composite Trapezoidal Rule, its principal error term is linear in the block size while the increased order and stability allow a modest increase in parallelism without further computational complexity. Numerical results confirm the enhanced properties of the higher-order method.

Keywords—Predictor-corrector methods, Ordinary differential equations, Parallel methods, Block methods.

1. INTRODUCTION

Several authors (see, for example, [1–9] and references therein) have considered block methods for the parallel solution of the initial value problem (IVP)

$$y' = f(t, y), \qquad y(t_0) = y_0, \tag{1}$$

where $y, f \in \mathbb{R}^s$. By means of a single application of a calculation unit, a block method yields a sequence of new estimates for y. If $k \geq 1$ is the block size, then in simple cases the values of t at which solutions are computed will be evenly separated. In other words, each basic cycle of the calculation has the potential to advance the solution by k new points in the t direction. Each such block can, therefore, be considered as a unit of calculation. Let y_n denote the approximation to the exact solution $y(t_n)$ at $t = t_n$. Also, f_n will denote the value of $f(t_n, y_n)$, the approximation for $y'(t_n)$. For $n = mk$, a block of solutions can be represented by the vector $Y_m = (y_{n+1}, y_{n+2}, \dots, y_{n+k})^{\mathsf{T}}$ with y_{n+j} $(1 \leq j \leq k)$, the generated solution at $t_{n+j} = t_n + jh$, where t_n is the right-hand end point of the preceding block and h is the uniform spacing between solution values. Adopting the notation of [7], the formula for the block method can be expressed

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$$Y_m = ey_n + hdf_n + hBF(Y_m), \tag{2}$$

where e and d are k-vectors, B is a $k \times k$ matrix, and F is a k-vector whose j^{th} entry is $f_{n+j} = f(t_{n+j}, y_{n+j})$, $1 \le j \le k$. As (2) is implicit in Y_m, it has to be solved iteratively using, in the first instance, predicted solution values. A predictor equation for Y can be expressed in the form

$$Y_m^{(0)} = ey_n + h\tilde{d}f_n, \tag{3}$$

where e and $\tilde{d}$ are k-vectors. Substitution of $Y_m^{(0)}$ into the right-hand side of (2) yields the block predictor-corrector (BPC) method

$$Y_m = ey_n + hdf_n + hBF\left(ey_n + h\tilde{d}f_n\right). \tag{4}$$

In accordance with the terminology used in the linear multistep case, this application is called PEC mode. Of course, one can continue this process by substituting the result of (4) into the right-hand side of (2) arriving at $P(EC)^\nu E^{1-\gamma}$ mode, in which $\gamma = 0$ indicates that a final evaluation is done before proceeding to the next block. Abbas and Delves [10] considered this approach using an explicit Euler predictor and then corrected twice by a trapezoidal corrector applied in the composition case. This method can be computed in three steps for each equidistant step point $r = 1, \dots, k$ as

$$\begin{aligned}
y_{n+r}^{(0)} &= y_n + rhf(t_n, y_n), \\
y_{n+r}^{(1)} &= y_n + \frac{h}{2}f(t_n, y_n) + h\sum_{i=1}^{r-1} f\left(t_{n+i}, y_{n+i}^{(0)}\right) + \frac{h}{2} f\left(t_{n+r}, y_{n+r}^{(0)}\right), \\
y_{n+r}^{(2)} &= y_n + \frac{h}{2} f(t_n, y_n) + h\sum_{i=1}^{r-1} f\left(t_{n+i}, y_{n+i}^{(1)}\right) + \frac{h}{2} f\left(t_{n+r}, y_{n+r}^{(1)}\right).
\end{aligned} \tag{5}$$

With $Y_m^{(0)}$ given by (3), method (5) has $P(EC)^2$ form

$$\begin{aligned}
Y_m^{(0)} &= ey_n + h\tilde{d}f_n, \\
Y_m^{(l+1)} &= ey_n + hdf_n + hBF\left(Y_m^{(l)}\right), \qquad l = 0, 1,
\end{aligned} \tag{6}$$

where

$$e = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}, \quad \tilde{d} = \begin{bmatrix} 1 \\ 2 \\ \vdots \\ k \end{bmatrix}, \quad d = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \vdots \\ \frac{1}{2} \end{bmatrix}, \quad B = \begin{bmatrix} \frac{1}{2} & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & \frac{1}{2} & 0 & \cdots & \cdots & 0 \\ & & \ddots & \ddots & & \vdots \\ 1 & \cdots & \cdots & 1 & \frac{1}{2} & 0 \\ 1 & \cdots & \cdots & 1 & 1 & \frac{1}{2} \end{bmatrix}.$$

While the local error of (6) has form

$$-\frac{kh^3}{12} y^{(3)}(t_n) + O\left(h^4\right), \tag{7}$$

an analysis of the $O(h^4)$ terms by Burrage [3] reveals a term of $((kh)^4/24)(f')^3 f$ thus, limiting the potential for massive parallelism. In this paper, we develop a fourth-order block scheme with the purpose of lessening this limitation somewhat, while improving the accuracy and linear stability properties of the method.

2. A BLOCK PREDICTOR-CORRECTOR SCHEME

In this section, we consider a block method in which the order is fixed but the block length may be any value at the cost of increasing the truncation error. The method developed uses equation (3) to predict solutions to the problem and then applies a corrector in $P(EC)^{\nu}E$ mode. The method can be written as

$$\begin{aligned} Y_{m+1}^{(0)} &= e \otimes y_n + h\,(A_p \otimes I)\,F\left(Y_m^{(\nu)}\right), \\ Y_{m+1}^{(l+1)} &= e \otimes y_n + h\,(A \otimes I)\,F\left(Y_{m+1}^{(l)}\right), \qquad l = 0, \dots, \nu - 1, \\ y_{m+1} &= e_{k+1}^{\top} Y_{m+1}^{(\nu)}, \end{aligned} \tag{8}$$

where

$$A_p = \begin{bmatrix} 0 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & 0 & \cdots & \cdots & \cdots & 1 \\ 0 & 0 & \cdots & \cdots & \cdots & 2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \cdots & \cdots & k \end{bmatrix}$$

is the $(k+1) \times (k+1)$ prediction matrix and $A = (\alpha_{i,j})$, $0 \le i,\ j \le k$ is the $(k+1) \times (k+1)$ Runge-Kutta matrix of coefficients. For starting purposes, we also take $Y_0^{(\nu)}$ to be the vector wherein, each of the $k+1$ components is y_0. With

$$A = \begin{bmatrix} 0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & \cdots & \cdots & \cdots & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} & 0 & \cdots & \cdots & 0 \\ \frac{1}{2} & 1 & 1 & \frac{1}{2} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{1}{2} & 1 & \cdots & \cdots & 1 & \frac{1}{2} & 0 \\ \frac{1}{2} & 1 & \cdots & \cdots & \cdots & 1 & \frac{1}{2} \end{bmatrix},$$

the block scheme (5) based on the composite Trapezoidal Rule arises, and in the sequel we will refer to it as TBPC when applied in $P(EC)^2E$ mode.

Our aim is to produce a fourth-order block scheme which might be very efficient to implement on parallel computers. As far as the order of accuracy is concerned, if we require a method of order p to be achieved then, as discussed in [11], the local truncation error will normally be of order $(kh)^{p+1}$, a very high dependence upon the block length k. For this reason, we construct a fourth-order parallel block predictor-corrector method for the numerical solution for IVP (1) based on the composite Simpson rule. In order to attain the desired accuracy, the matrix of coefficients A in (8) must satisfy the following equations for $r = 1, 2, \ldots, k$:

$$\begin{aligned} \sum_{j=0}^{k} \alpha_{r,j} &= r, \\ \sum_{j=0}^{k} j\alpha_{r,j} &= \frac{r^2}{2}, \\ \sum_{j=0}^{k} j^2\alpha_{r,j} &= \frac{r^3}{3}, \\ \sum_{j=0}^{k} j^3\alpha_{r,j} &= \frac{r^4}{4}. \end{aligned} \tag{9}$$

For $k = 4$, a solution of the order equations (9) based on the composite Simpson rule has Runge-Kutta matrix

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \frac{3}{8} & \frac{19}{24} & \frac{-5}{24} & \frac{1}{24} & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{1}{3} & 0 & 0 \\ \frac{3}{8} & \frac{9}{8} & \frac{9}{8} & \frac{3}{8} & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{1}{3} \end{bmatrix},$$

while with $k = 10$, the corresponding coefficient matrix becomes

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{8} & \frac{19}{24} & \frac{-5}{24} & \frac{1}{24} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{8} & \frac{9}{8} & \frac{9}{8} & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{17}{24} & \frac{9}{8} & \frac{9}{8} & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{17}{24} & \frac{9}{8} & \frac{9}{8} & \frac{3}{8} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{17}{24} & \frac{9}{8} & \frac{9}{8} & \frac{3}{8} & 0 \\ \frac{1}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{2}{3} & \frac{4}{3} & \frac{1}{3} \end{bmatrix}. \tag{10}$$

In the next section, we investigate the accuracy and linear stability properties of this block scheme which we denote by SBPC when applied in $P(EC)^4E$ mode.

3. ACCURACY AND STABILITY

With four applications of the corrector, the principal local truncation error of SBPC is that of the corrector. The k^{th} component of the principal local truncation error is then given by

$$\epsilon_k = y(t_{n+k}) - y(t_n) - h\sum_{j=0}^{k} \alpha_{k,j} y'(t_{n+k}). \tag{11}$$

For k even, expansion of (11) yields

$$\begin{aligned}\epsilon_k &= \left[\frac{k^5h^5}{120} - \frac{h^5}{72}\left(4(1^4+3^4+5^4+7^4+\cdots+(k-1)^4)\right.\right.\\ &\quad \left.\left. + 2\left(2^4+4^4+6^4+\cdots+(k-2)^4\right) - \frac{k^4h^5}{72}\right] y^{(5)}(t_n),\\ &= -\frac{kh^5}{180}\, y^{(5)}(t_n),\end{aligned} \tag{12}$$

with the same result for k odd. From (12), the principal error is only linear in the block size k, and consequently, offers the potential for massive parallelism. However, analogous to the investigation by Burrage [3] regarding the second-order block method of Abbas and Delves [10], the $O(h^6)$ terms in the local error finally dominate the principal error term since a term with coefficient $((kh)^6/6!)$ surfaces. While this indeed limits the potential parallelism, it is certainly a less modest limitation.

The linear stability properties of the block corrector formula (8) are determined through application to the test equation

$$y' = \lambda y, \qquad \lambda < 0. \tag{13}$$

Letting $z = \lambda h$, in the case $k = 4$, (8) becomes

$$\begin{bmatrix} 1-\frac{19}{24}z & \frac{5}{24}z & \frac{-1}{24}z & 0\\ -\frac{4}{3}z & 1-\frac{1}{3}z & 0 & 0\\ -\frac{9}{8}z & -\frac{9}{8}z & 1-\frac{3}{8}z & 0\\ -\frac{4}{3}z & -\frac{2}{3}z & -\frac{4}{3}z & 1-\frac{1}{3}z \end{bmatrix} \begin{bmatrix} y_{n+1}\\ y_{n+2}\\ y_{n+3}\\ y_{n+4}\end{bmatrix} = \begin{bmatrix} 1+\frac{3}{8}z\\ 1+\frac{1}{3}z\\ 1+\frac{3}{8}z\\ 1+\frac{1}{3}z\end{bmatrix} y_n.$$

With

$$Q = \begin{bmatrix} 1-\frac{19}{24}z & \frac{5}{24}z & \frac{-1}{24}z & 0\\ -\frac{4}{3}z & 1-\frac{1}{3}z & 0 & 0\\ -\frac{9}{8}z & -\frac{9}{8}z & 1-\frac{3}{8}z & 0\\ -\frac{4}{3}z & -\frac{2}{3}z & -\frac{4}{3}z & 1-\frac{1}{3}z \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} 1+\frac{3}{8}z\\ 1+\frac{1}{3}z\\ 1+\frac{3}{8}z\\ 1+\frac{1}{3}z\end{bmatrix},$$

using Cramer's rule, we find that

$$y_{n+r} = \frac{D_r(z)}{D(z)}\, y_n, \qquad r = 1,2,3,4,$$

where $D(z) = \det(Q)$ and $D_r(z) = \det(Q_r)$, and Q_r is obtained from Q by replacing its r^{th} column by the vector b. Absolute stability then requires

$$\left|\frac{D_r(z)}{D(z)}\right| < 1. \tag{14}$$

Of course, in general, absolute stability properties depend on the predictor and the mode of implementation. Applying (8) with ν corrections to the standard linear test problem (13) yields $Y_{m+1}^{\nu} = T^m(z)Y_0^{\nu}$, where with

$$E = \begin{bmatrix} 0 & 0 & \cdots & \cdots & \cdots & 1 \\ 0 & 0 & \cdots & \cdots & \cdots & 1 \\ 0 & 0 & \cdots & \cdots & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \cdots & \cdots & 1 \end{bmatrix},$$

the stability matrix $T(z)$ is given by [3]

$$T(z) = E + \sum_{j=1}^{\nu} A^j E z^j + z^{\nu+1} A^{\nu} A_p. \tag{15}$$

Consequently, the stability boundary is the largest number α such that if $z \in (-\alpha, 0)$, then $\rho(T(z)) < 1$, where $\rho(T(z))$ denotes the spectral radius of $T(z)$. Since $A^{\nu}A_p = ue_{k+1}^{\mathrm{T}}$,

$$\rho(T(z)) = \left| 1 + kz + \cdots + \frac{(kz)^{\nu}}{\nu!} + u_{k+1}(kz)^{\nu+1} \right|.$$

Taking $\nu = p$, where p is the order of the block method, a little algebra reveals that

$$\rho(T(z)) = \left| 1 + kz + \cdots + \frac{(kz)^p}{p!} + \left(\frac{1}{(p+1)!} - \frac{C_{p+1}^k}{k^{p+1}} \right) (kz)^{p+1} \right|, \tag{16}$$

where C_{p+1}^k is the error constant of the method at the k^{th} point in the block. In this case, the stability polynomial is simply a perturbation of that corresponding to a $(p+1)^{\text{th}}$ order explicit Runge-Kutta method scaled according to block size. Table 1 contains the values of α_T and α_S of block predictor-corrector schemes in $P(EC)^{\nu}E$ mode, based on composite Trapezoidal and Simpson Rules, respectively. Corresponding to $\nu = \infty$, we have also included in Table 1 the stability boundaries of the correctors obtained from (14), and its analogues to other block sizes and schemes based on the composite Trapezoidal Rule. The error constants for TBPC and SBPC are $C_3^k = -(k/12)$ and $C_5^k = -(k/180)$, respectively. Consequently, from (16) with increasing k, the interval of stability of TBPC quickly approaches that of scaled explicit third-order Runge-Kutta methods which is approximately $((-2.5127/k), 0)$. Similarly, the interval of stability of SBPC approaches that of scaled explicit fifth-order Runge-Kutta methods which is approximately $((-3.2170/k), 0)$.

Table 1. Stability boundaries.

k	ν	α_T	α_S
4	2	0.6161	0.6282
	4	0.7483	0.8033
	6	0.8608	0.9639
	8	0.9544	1.0537
	∞	∞	7.4225
10	2	0.2505	0.2512
	4	0.3175	0.3217
	6	0.3842	0.3952
	8	0.4477	0.4690
	∞	∞	3.0716

4. NUMERICAL RESULTS

We first consider the nonlinear IVP

$$y' = -\frac{y^3}{2}, \qquad y(0) = 1, \tag{17}$$

for $t \in [0,4]$ with exact solution $y = 1/\sqrt{t+1}$. Table 2 contains the maximum absolute errors using the TBPC and SBPC methods with block sizes $k = 4$ and $k = 10$ with various step sizes. Letting e_1 and e_2 be the maximum absolute errors at $t = 4$ using step sizes h_1 and h_2, respectively, and assuming that $e_i = Ch_i^p$. Table 2 also includes the observed rates of convergence calculated using $p = (\ln(e_1/e_2)/\ln(h_1/h_2))$. For problem (17), at least second-order accuracy is apparent for TBPC and fourth-order accuracy for SBPC. In addition, a visual analysis reveals the effect of the linear dependency of the principal local truncation error on the block size.

Table 2. Approximate rate of convergence.

k	h	TBPC	p	SBPC	p
4	0.2	$0.1004E-01$	–	$0.2264E-03$	–
	0.1	$0.1256E-02$	3.00	$0.8941E-05$	4.66
	0.05	$0.1824E-03$	2.78	$0.2980E-06$	4.91
10	0.2	$0.9995E-01$	–	$0.9173E-02$	–
	0.1	$0.1690E-01$	2.56	$0.5959E-03$	3.94
	0.05	$0.2033E-02$	3.06	$0.2390E-04$	4.64

To numerically investigate the linear stability properties of the block predictor-corrector schemes we next consider the linear IVP

$$y' = -100\,(y - \sin(t)) + \cos(t), \qquad y(0) = 0, \tag{18}$$

for $t \in [0,1]$ with exact solution $y = \sin(t)$. Table 3 contains the maximum absolute errors using the TBPC and SBPC methods with block sizes $k = 4$ and $k = 10$, with several step sizes near the stability boundaries. For problem (18), with $k = 4$, this approximately translates to $h < 0.0062$ and $h < 0.0080$ for TBPC and SBPC, respectively, while with $k = 10$, they become $h < 0.0025$ and $h < 0.0032$ for TBPC and SBPC, respectively. The increased stability of the higher-order method SBPC is clearly evident in Table 3.

Table 3. Maximum absolute error.

k	h	TBPC	SBPC
4	$\frac{1}{180}$	$0.5841E-04$	$0.1401E-04$
	$\frac{1}{160}$	$0.8071E-04$	$0.2462E-04$
	$\frac{1}{140}$	$0.2797E+03$	$0.4363E-04$
	$\frac{1}{120}$	$0.7598E+08$	$0.6955E-03$
	$\frac{1}{100}$	$0.1547E+14$	$0.1950E+08$
10	$\frac{1}{400}$	$0.7039E-04$	$0.2420E-04$
	$\frac{1}{360}$	$0.1514E+01$	$0.3821E-04$
	$\frac{1}{320}$	$0.2788E+06$	$0.5859E-04$
	$\frac{1}{300}$	$0.3504E+08$	$0.5947E-03$
	$\frac{1}{280}$	$0.3948E+09$	$0.2269E+02$

5. CONCLUSION

In this paper, we have presented a one step fourth-order explicit block method which can utilize an arbitrary number of concurrent processors. While the higher-order truncation error terms eventually dominate the error with increasing block size, they do so at a slower rate than that of a second-order block method based on the composite Trapezoidal rule, thereby allowing a higher degree of parallelism. While two additional corrections are required in the fourth-order scheme, the same number of corrections applied to the second-order scheme still results in a smaller interval of absolute stability and, of course, leaves the method second-order.

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